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Caution about evolving program versions

This part of the user guide is based on an initial user manual from November 2014 for the SweetUnityMol version of our software. It is currently being adapted and updated to match the current development builds of the 0.9.5 series. In the meantime, several descriptions and screen captures may still pertain to previous versions of the software and may be inaccurate for the current builds. Please be aware of this limitation.

Warning : Screenshots and examples in this document may differ from the current UnityMol version

References

Zhihan Lv, Alex Tek, Franck Da Silva, Charly Empereur-mot, Matthieu Chavent, Marc Baaden **Game on, Science - how video game technology may help biologists tackle visualization challenges** *PLoS ONE* 6 mars 2013, 8(3): e57990. doi:10.1371/journal.pone.0057990

Serge Perez, Thibault Tubiana, Anne Imberty, Marc Baaden, **Three-dimensional representations of complex carbohydrates and polysaccharides--SweetUnityMol: a video game-based computer graphic software.** *Glycobiology*. 2015, 25(5):483-91. doi: 10.1093/glycob/cwu133.

Installing the software

The software described below has been initially developed based on revision 676 of UnityMol and version 4.5.2f1 of Unity3D. All source code was implemented using C# and Cg languages built into Unity 3D and is available along with executables for Mac, Windows and Linux platforms on the sourceforge project website. Current UnityMol versions run within version 5.3.2f1 of Unity3D.

<https://sourceforge.net/projects/unitymol/files/>

Further documentation, input files, and series of illustrations can be found at

<http://glycopedia.eu/IMG/pdf/unitymol-user-manual.pdf>

and in the online UnityMol doxygen documentation available from

<http://www.baaden.ibpc.fr/umol/Doc/manual/html/pages.html>

Windows version (2014/10/02)

- 32 bits
 - umol-win32-20141002_Data
 - Run_SweetUmol_32.bat
 - umol-win32-20141002.exe
- 64 bits
 - umol-win64-20141002_Data
 - Run_SweetUmol_64.bat
 - umol-win64-20141002.exe

Note. This part and the following need to be updated to version 0.9.5

Mac version (2014/10/02)

- umol-macosx-universal-20141002.app

Linux version (2014/10/02)

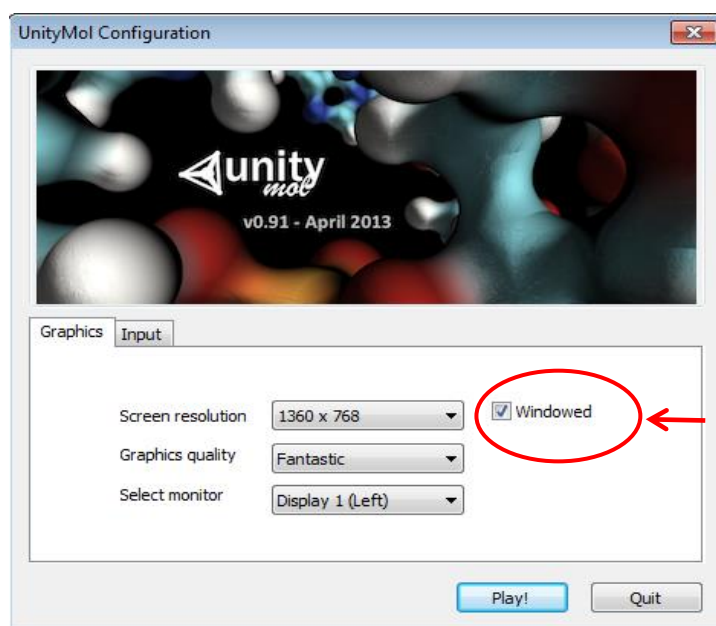
- umol-linux-20141002_Data
- umol-linux-20141002.x86
- umol-linux-20141002.x86_64

Version July 2016

Running the 32 and 64 bits Windows version

Start the program before loading any atomic coordinate files.

If you encounter issues running UnityMol, try to **NOT USE THE FULL SCREEN MODE** (check `Windowed` in the "UnityMol Configuration" menu (this menu is the menu where you set the resolution and click on `Play!`)).

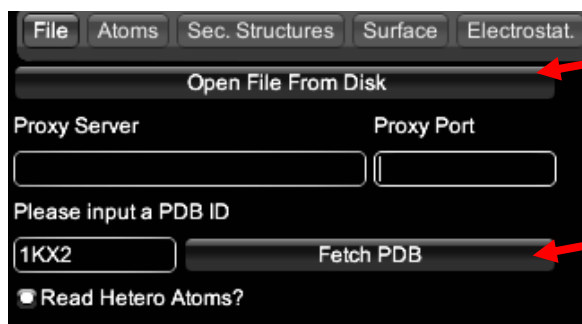


Main menu



The menu bar sits on the top and groups several submenus together that are described hereafter. Some of these options offering advanced visualization and manipulations (haptic arm) are being implemented and are not functional at this time: November 2014.

1 File menu : PDB Loading



1 – Open a file from hard drive (you can't change hard drive yet).

UnityMol and the *pdb* file have to be on the same drive but on different directories).

2 – Fetch a *pdb* from the *pdb* database (if "Proxy Server" and "Proxy Port" are not empty, please remove all fields

By default the visualization of UnityMol is the Particle mode. This mode uses the particle system of Unity3D to display the molecule. This may not be the most appropriate visualization. Changing to SmoothHyperballs mode offers a better visualization (this setting is the default option in more recent builds of UnityMol).

2 Atom



Different types of representations are available by **Atom** (1) or by **Bond** (2).

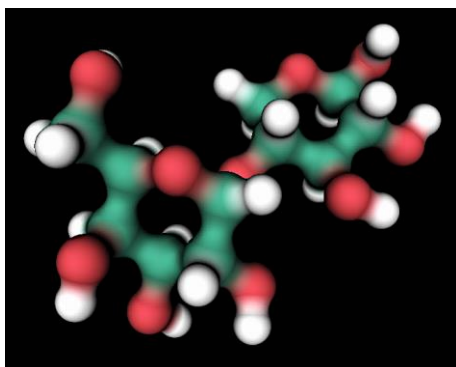
The preselected visualization called **Hyperball** (3), the most interesting one (Figure above).

The **Renderer** (4) and **Panels** (5) menus are made to change the **color** and the **texture** of either the entire molecule, or a selection.

Hide: Hide the molecule (this option is activated when some visualization option (like secondary structures) is activated. Uncheck this box to display both the secondary structure and the molecule.

Radius: Change the radius of atom spheres.

LOD mode: When in the Hyperballs mode and this option is checked (and upon changing the orientation of the camera) the molecule will be displayed in the *particle* mode prior recreating the Hyperball representation. This is to be used for large macromolecular systems for which the Hyperballs representation reduces frame rate too much. FPS: Frame Per Second.



Automove (or **SPACE** key): the camera will turn around the molecule.

Lock Camera: The camera will not be able to move when this option is checked.

Brightness : Adjust the brightness of Hyperballs. This is useful for some dark textures, or when using texture grayscale plus added colors.

Hyperball Visualization

A – HyperBall Style menu



Shrink: To adjust the shape of the bond

Scale: To adjust the scale of the bond

Dfactor: Only for Biological Networks

Metaphor: Pre-configured style (CPK, Licorice, VdW, Smooth Hyperballs)

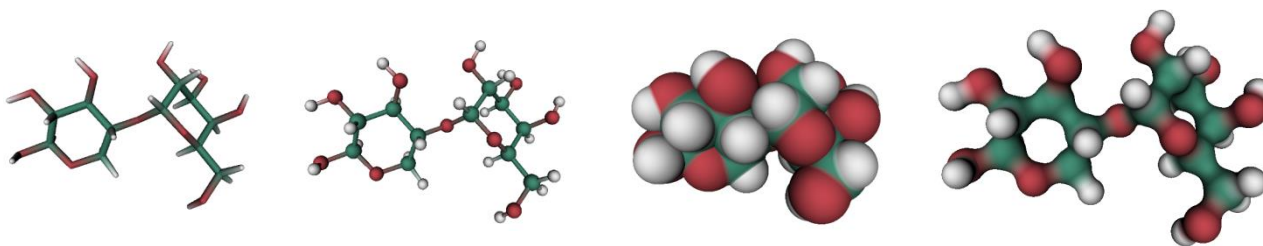
Interactive mode: Use spring forces to make an interactive molecule (an atom can be dragged and it will go back to its original position).

Drag/Spring: Spring parameters for interactive mode.

Velocity Colors: Colors each atom in interactive mode from white (slow) to black (very fast) based on the velocity of each particle.

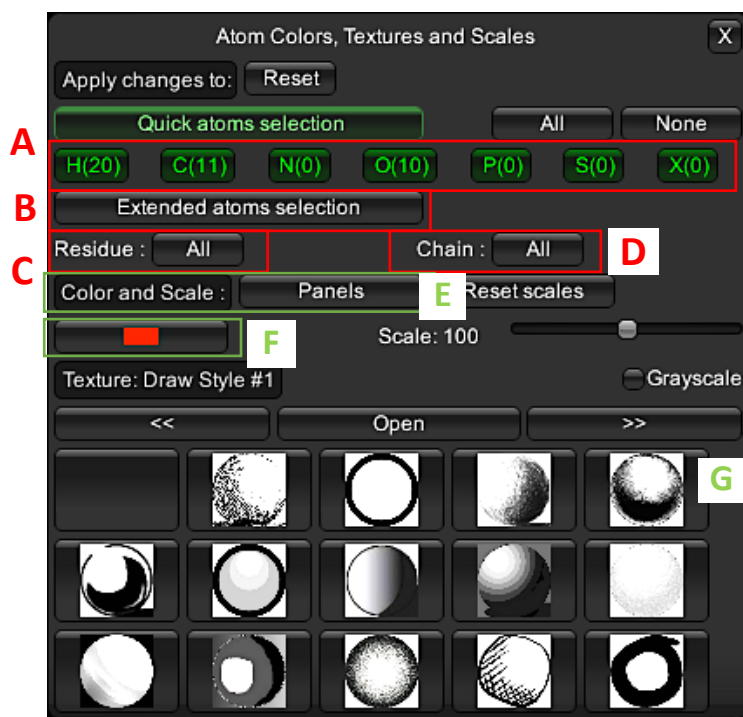
Measure dist.: Activate and click on 2 atoms to display their distance.

Dist. Cueing: Adjust the light according to the distance of the camera.



Example rendering of Ball & Sticks, Licorice, VdW, Smooth Hyperballs metaphors

B – Render Menu (4)



The whole molecule is selected by default. The selection can be changed by:

- Atom Type (A)
- Atom name (B)
- Residue name (C)
- By chain (D)

The selection can be combined.

Pre-configured coloration is on the **Panels** menu (E). Another color can be selected by clicking on the Color Button (F).

A texture can be selected and applied to the selection (G). Several textures are available on other pages (you can switch pages by clicking << and >>).

C – Panels Menu (3)



This menu contains pre-configured colors. You can switch by clicking on the buttons.

Color Panels:

- **All white:** make the molecule all white.
- **Goodsell:** make the color softer.
- **WaterColor:** color carbons in blue.
- **Pastel:** default colors.
- **CPK:** color with the CPK color code.
- **Basic:** color carbon in green.
- **IUPAC:** color with the IUPAC color code.
- **Chains:** color by chain
- **Sugar:** color by sugar Type (the molecule must contain sugar).
- **ADN/ARN:** coloration for DNA and RNA.

Texture Panels:

- **Default:** default texture
- **CPK:** CPK coloration with adapted texture.
- **Acid-Basic:** coloration and texture according to the acid-basic status of amino acids.

3 Secondary Structures

Secondary Structures

Secondary structures

☐ Enable Secondary structures

Helix Width: 1.50

Sheet Width: 1.70

Coil Width: 0.30

Thickness: 0.30

Helix diameter: 1.80

Arrow width: 1.80

Color by ss

Color by chain

Apply changes

C-alpha trace

☐ C-alpha trace

Smoothness

Bfactor Representation

B Factor

Smoothness

Choose scale Min Max

Rescaling Reset

High value radius

Activate the Secondary Structure visualization.

Adjust parameters for the secondary structure visualization.

Color by secondary structure type.

Color by chain type.

Don't forget to **click on this button to apply changes**.

Trace the shape of the proteins by a spline passing by all carbon alpha. Smoothness is used to adjust the smoothness of the trace.

Like the C-alpha trace, but adjust the radius and the color of each sphere with the B factor value.

Adjust the scale of the B-factor used.

4 Surface



T: Density threshold used to generate the isosurface

Generate: generate the surface.

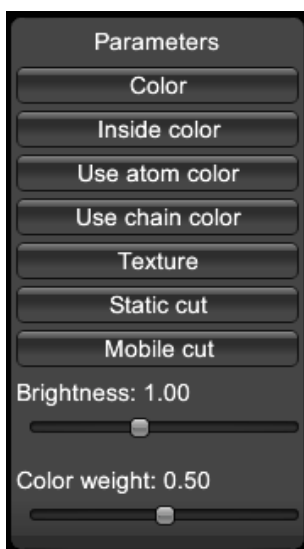
BFactor: adjust the shape of the surface according to the bfactor value.

Volumetric: show the volumetric space of the protein with a particle system.

Toggle surface: hide surface representation (when you change a parameter, you have to hide the surface and press the *Generate* button again).

HetAtoms/Sugars: show surface for HetAtoms or and Sugar molecules

Upon selecting the *Generate* button, this window will appear.



Color: change the color of the surface (external face).

Inside color: change the inside color.

Use atom color: Color the surface according to the type of atom under each portion of it.

Use chain color: use the color of the chains.

Texture: apply a texture on the surface.

Static cut: cut the surface (you can control the cutting by a pad that will appear in the upper right corner).

Mobile cut: cut the surface and the cut will be the same when you change the camera's orientation.

Brightness: adjust the brightness of the surface

Color weight: adjust the color concentration on the surface.

5 Electrostatic

To use this menu, the following files have to be set in the same folder: the PDB file (and the same name) a file with extension ".dx" and ".apf" generated with softwares such as APBS (A wide-spread software for evaluating the electrostatic properties of biomolecular systems).



Transparency: Add transparency to the mesh generated when you load the negative and positive electrostatic visualization.

T: Threshold used to generate the electrostatic isosurface.

Load Neg/Pos: load electrostatic visualization.

Toggle Neg/Pos: show or hide the electrostatic visualization.

Volumetric Fields: volume rendering of the electrostatic fields.

Field Lines: show the Field Lines visualization (examine the local intensity of electric fields).

6 Display

This menu is made **to take screenshot**, change the background and add special effects.



Screenshot (or P key): take a screenshot

ScreenShot Sequence: doesn't work yet.

Background: add a picture in the background (switch between yes/no)

White/Gray/Black: quick selection of background color

Background Color: choose your background color with a color panel.

Effects: add special effect.

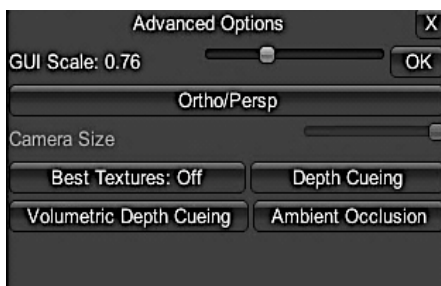
Infos: show/hide FPS info and Atom/Bond number.

List of all visual effects:

- SSAO** Screen Space Ambient Occlusion. Works on spheres, cubes, surfaces and secondary structures
- DOF** Focus on a point and make fuzzy all atoms far away from this point. This effect requires selecting (by clicking) an atom. It works better for large molecules.
- EDGE** The edge of every atom is black.
- CREASE** Add a thick contour to the molecule.
- SEPIA** Use a SEPIA coloration.
- GRAYS** Make the molecule black and white.
- GLOW** Make all atoms shiny.
- BLUR** Add a blur effect upon moving the camera.
- NOISE** Add noise on the screen
- BLUR2** Constant blur.
- VORTEX** Twist the molecule around the center.
- TWIRL** Similar to VORTEX

7 Advanced

This menu offers advanced options (some are being implemented).



GUI Scale: change the size of the GUI.

Ortho/Persp: doesn't work yet.

Best Textures: don't use anymore.

Depth Cueing: doesn't work yet.

Volumetric Depth Cueing: Doesn't work yet.

Ambient Occlusion: darkens the densest parts of the molecule to improve depth perception.

8 Guided Navigation

This menu is used to make a “guided navigation”, but for now it works only with the pdb 3E10 (GLIC) as part of work in progress.



Symmetry origin: X,Y,Z coordinates of the center of symmetry.

Symmetry direction: vector of the symmetry direction.

Send: activate the guided navigation mode.

9 Sugar

This menu is made to deal with the specific features of sugar visualization (principally made with the POLYS 2.0 software. But the visualization mode called *Ring Blending* works with all molecules.



Enable Ring Blending: enable the filling of all rings (aromatic, sugar, or other cycle) with a semi transparent color.

Enable SugarRibbons: enable the SugarRibbons visualization (to transform a sugar into a “schematic” representation like secondary structures, but adapted for sugars).

Hide Hydrogens: hide hydrogen atoms

Sugar /Non Sugar : hide non sugar atoms



Tune Menu

Show Oxygens: to display the intracyclic oxygen atom as a sphere.

Sugar Only : To adjust the size of the radius of the sphere.

Ribbons Thickness: to adjust the thickness of the ribbon.

Inner Ring Thickness: to adjust the thickness of the ring.

Outer Ring Thickness: to adjust the thickness of the ring.

Pyranose: to adjust the thickness of the glycosidic bond (for pyranose)

Pyranose: to adjust the thickness of other bonds (for pyranose)

Furanose: to adjust the thickness of the other bonds (for furanose)

Note. Do not forget to click on “Apply changes” button to apply the selected new parameters.



Tune submenu

For Oxygen Sphere, Outer Rings and Bond:

Sugar : use the sugar color to color Oxygen/Outer Rings or Bonds.

Chain : use the chain color to color Oxygen/Outer Rings or Bonds

Custom color : open a color picker windows to choose a custom color for Oxygen/Outer Rings or Bonds.

The color can be made darker or lighter with the Light Color Factor slider.

Note. « Apply Changes » button is **not needed** for this feature.

10 VRPN

This menu is used to connect a **haptic arms**, but you need a VRPN server installed on your computer. Work in progress.

11 MDDriver

This menu is used to connect a molecular simulation in real-time. Work in progress.

12 Reset

Reset the view.

General

Binding Keys

Key to press	Action to carry out
LEFT Arrow – A	Move LEFT
RIGHT Arrow – D	Move RIGHT
DOWN arrow - S	Move DOWN
UP arrow – W	Move UP
Q	Rotation DOWN
E	Rotation UP
Z	Rotation LEFT
X	Rotation Right
N	ZOOM +
B	ZOOM –
P	Screenshot (only on local pdb; doesn't work yet on fetched PDB)
BACKSPACE	Hide GUI
SPACE	Automove (rotation right)
R	Reset to center
C	Center to one or several atoms (select an atom/group with the selection mode first).

Guided Navigation (only for 3EI0)

These controls are only available when Guided Navigation mode is activated. The actual version is specific to pentameric channels (especially the PDB file 3EI0).

Constrained navigation

Key to press	Action to carry out
U	Enable/Disable automatic Constrained Navigation UP (panoramic mode)
J	Enable/Disable automatic Constrained Navigation DOWN (panoramic mode)
UP ARROW - W	Constrained Navigation Up
DOWN ARROW - S	Constrained Navigation Down
RIGHT ARROW - D	move RIGHT
LEFT ARROW - A	move LEFT

Spreading

This mode doesn't work for particles and cubes. Second step is only available by fetching PDB 3EI0.

Key to press	Action to carry out
Numpad + or B	Spreading chains
Numpad - or V	Narrowing chains
Numpad * or T	Reset chains
L	Enable/Disable spreading near the structure (active by default)

Panoramic mode

Key to press	Action to carry out
I	Enable/Disable panoramic mode
LEFT ARROW - A	turn LEFT
RIGHT ARROW - D	turn RIGHT
DOWN ARROW - S	move DOWN
UP ARROW - W	move UP

Monomer jump mode

Key to press	Action to carry out
M	Enable/Disable monomer jump mode
LEFT ARROW - A	Next monomer on left
RIGHT ARROW - D	Next monomer on right

Input File generated by SWEET

Version July 2016

Input File generated by POLYS (Starch Double Helical Structure)

	3letter Sugar code	Chain ID	Residue Number		
ATOM	1 C1	GLC A	1	2.145	-3.715
ATOM	2 C2	GLC A	1	0.918	-4.595

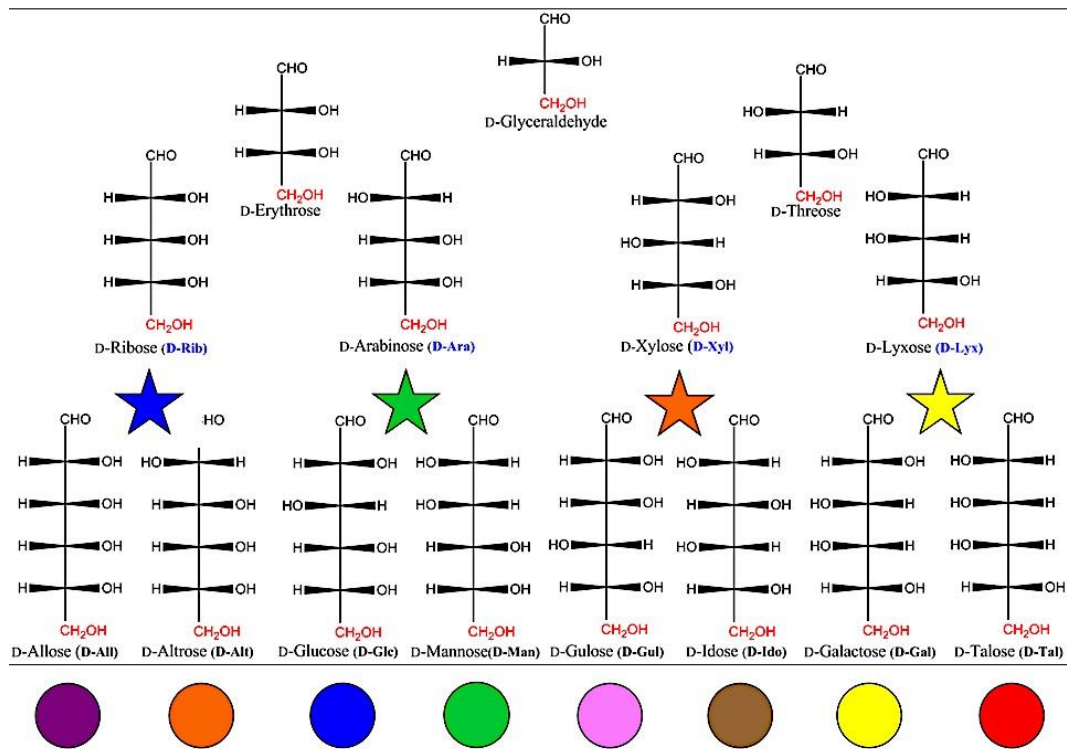
```

1 ATOM 1 C1 GLC A 1 2.145 -3.715 3.129 1.00 0.00
2 ATOM 2 C2 GLC A 1 0.918 -4.595 2.908 1.00 0.00
3 ATOM 3 C3 GLC A 1 -0.334 -3.978 3.523 1.00 0.00
4 ATOM 4 C4 GLC A 1 -0.058 -3.703 4.999 1.00 0.00
5 ATOM 5 C5 GLC A 1 1.189 -2.828 5.142 1.00 0.00
6 ATOM 6 C6 GLC A 1 1.589 -2.597 6.600 1.00 0.00
7 ATOM 7 O1 GLC A 1 1.983 -2.496 2.397 1.00 0.00
8 ATOM 8 O2 GLC A 1 0.715 -4.752 1.496 1.00 0.00
9 -----
10 ATOM 214 C1 GLC B 11 -3.715 2.145 1.564 1.00 0.00
11 ATOM 215 C2 GLC B 11 -3.093 3.520 1.344 1.00 0.00
12 ATOM 216 C3 GLC B 11 -1.699 3.613 1.959 1.00 0.00
13 ATOM 217 C4 GLC B 11 -1.801 3.236 3.434 1.00 0.00
14 ATOM 218 C5 GLC B 11 -2.444 1.855 3.577 1.00 0.00
15 ATOM 219 C6 GLC B 11 -2.675 1.455 5.035 1.00 0.00
16 ATOM 220 O1 GLC B 11 -2.965 1.171 0.832 1.00 0.00
17 ATOM 221 O2 GLC B 11 -2.995 3.758 -0.068 1.00 0.00
18 ATOM 222 O3 GLC B 11 -1.264 4.978 1.894 1.00 0.00

```


Sugar ring color code for monosaccharides

Symbol Nomenclature for Glycans (SNFG) Varki et al., *Glycobiology*, 2015, 25, 12, 1323-1324 *



White (Generic)	Blue	Green	Yellow	Orange	Pink	Purple	Light Blue	Brown	Red
Hexose ○	Glc ●	Man ●	Gal ●	Gul ●	Alt ●	AlI ●	Tal ●	Ido ●	
HexNAc □	GlcNAc ■	ManNAc ■	GalNAc ■	GulNAc ■	AltNAc ■	AlINAc ■	TalNAc ■	IdoNAc ■	
Hexosamine ◻	GlcN ◻	ManN ◻	GalN ◻	GulN ◻	AltN ◻	AlIN ◻	TalN ◻	IdoN ◻	
Hexuronate ◇	GlcA ◇	ManA ◇	GalA ◇	GulA ◇	AltA ◇	AlIA ◇	TalA ◇	IdoA ◇	
Deoxyhexose △	Qui ▲	Rha ▲			6dAlt ▲		6dTal ▲		Fuc ▲
DeoxyhexNAc △	QuiNAc ▲	RhaNAc ▲							FucNAc ▲
Di-deoxyhexose ◻	Oli ■	Tyv ■		Abe ■	Par ■	Dig ■	Col ■		
Pentose ☆		Ara ★	Lyx ★	Xyl ★	Rib ★				
Nomiosonate ◇		Kdn ◇				Neu5Ac ◇	Neu5Gc ◇	Neu ◇	
Unknown ◻	Bac ●	LDManHep ●	Kdo ●	Dha ●	DDManHep ●	MurNAc ●	MurNGc ●	Mur ●	
Assigned ◻	Api ●	Fru ●	Tag ●	Sor ●	Psi ●				

(*) Ajit Varki, Richard D Cummings, Markus Aebi, Nicole H Packer, Peter H Seeberger, Jeffrey D Esko, Pamela Stanley, Gerald Hart, Alan Darvill, Taroh Kinoshita, James J Prestegard, Ronald L Schnaar, Hudson H Freeze, Jamey D Marth, Carolyn R Bertozzi, Marilyn E Etzler, Martin Frank, Johannes FG Vliegthart, Thomas Lütke, Serge Perez, Evan Bolton, Pauline Rudd, James Paulson, Minoru Kanehisa, Philip Toukach, Kiyoko F Aoki-Kinoshita, Anne Dell, Hisashi Narimatsu, William York, Naoyuki Taniguchi, Stuart Kornfeld, **Symbol nomenclature for graphical representations of glycans**, *Glycobiology*, 2015, 25, 12, 1323-1324

Color code for monosaccharides

3 letter code	Colour
6DAL	Pink
6DTA	Light Blue
ABE	Orange
ALL	Purple
ALT	Pink
API	Blue
ARA	Green
BAC	Blue
COL	Light Blue
DDM	Pink
DHA	Orange
DIG	Purple
FRU	Green
FUC	Red
GAL	Yellow
GLC	Blue
GUL	Orange
IDO	Brown
KDN	Green
KDO	Yellow

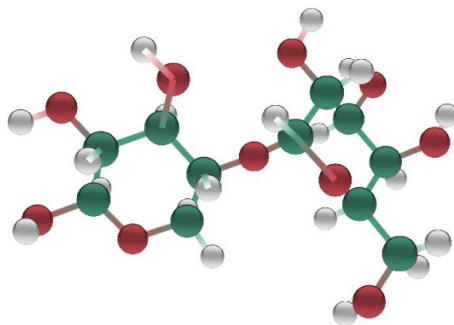
3 letter code	Colour
LDM	Green
LYX	Yellow
M5A	Purple
M5C	Light Blue
MAN	Green
MUR	Brown
N5G	Light Blue
NEU	Brown
OLI	Blue
PAR	Pink
PSI	Pink
QUI	Blue
RHA	Green
RIB	Pink
SIA	Purple
SOR	Orange
TAL	Light Blue
TYV	Green
XYL	Orange

3 letter code	Colour
BLU	Blue
GRE	Green
YEL	Yellow
ORA	Orange
PIN	Pink

3 letter code	Colour
PUR	Purple
LBL	Light Blue
BRO	Brown
RED	Red
GRE	Grey

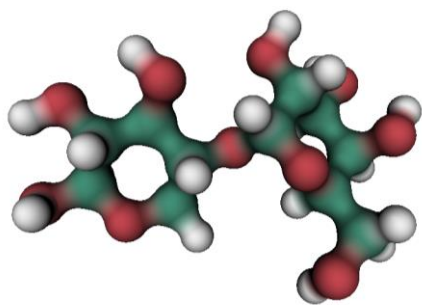
Examples

Particles mode

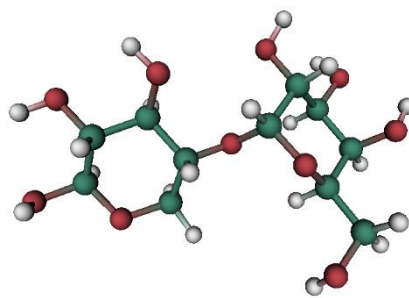


Smooth HyperBalls mode

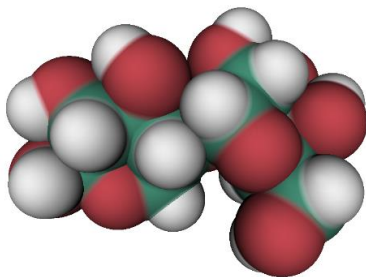
Default Smooth HyperBalls mode



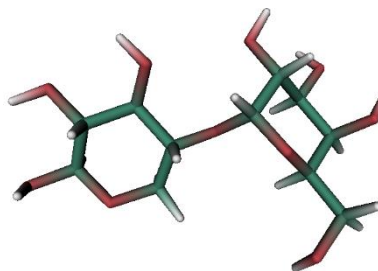
CPK mode



Van der Waals

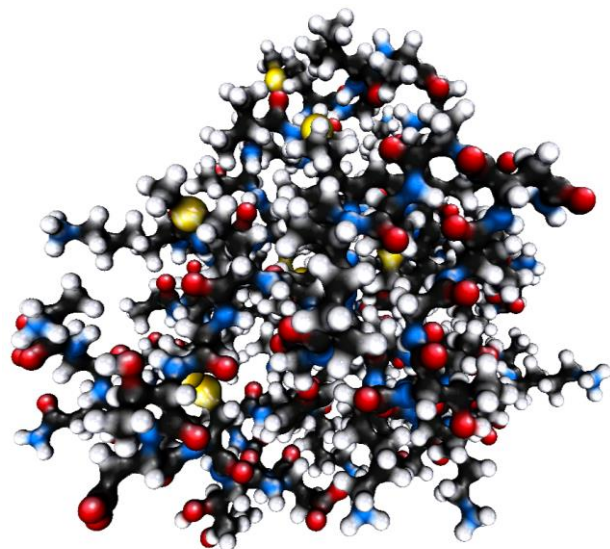


Licorice

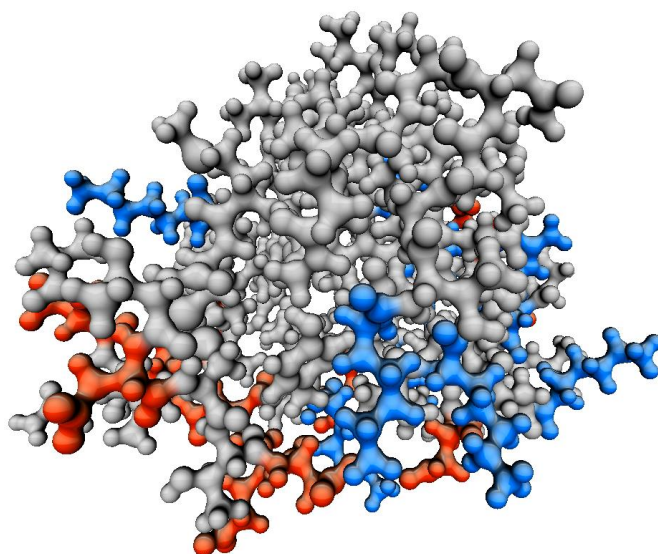


Texture

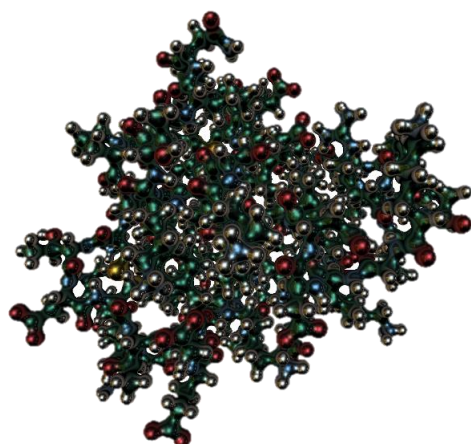
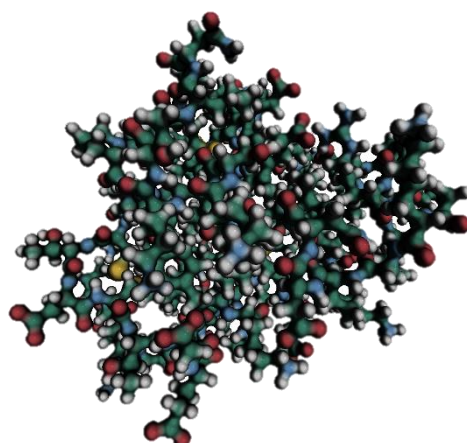
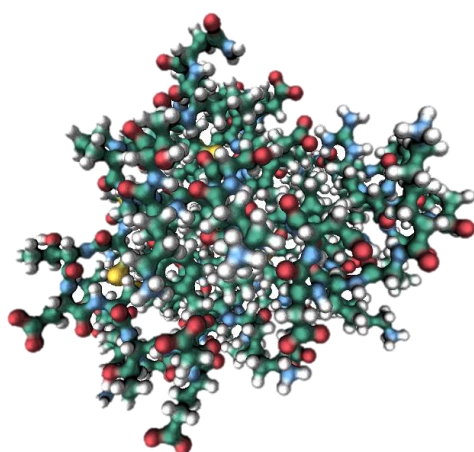
CPK



Acid-Basic

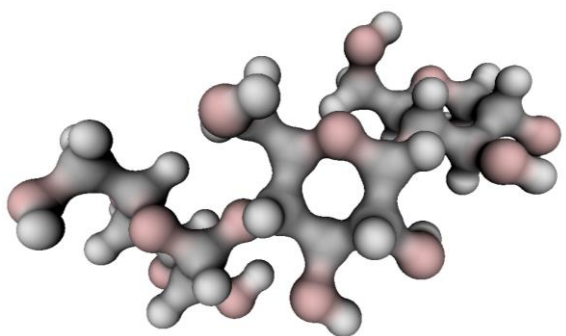


*Other examples
(Renderer Menu)*

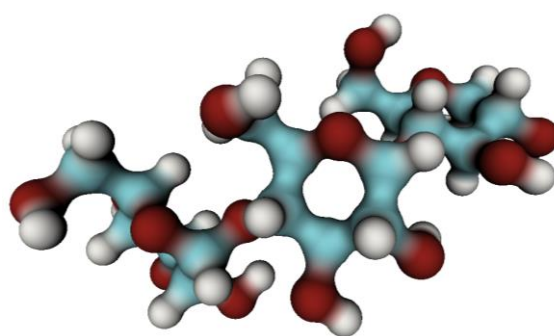


Coloration Mode

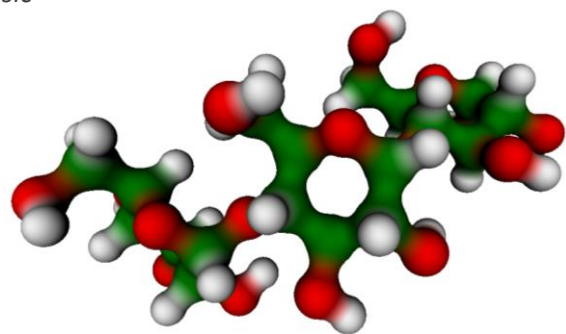
GoodSell



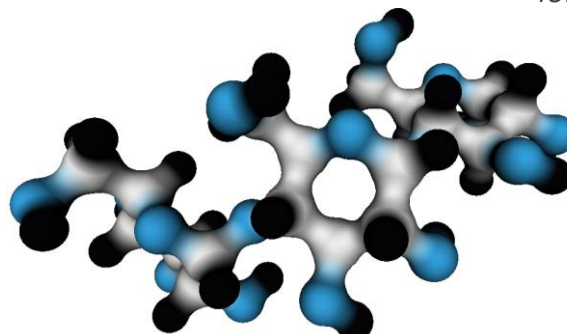
WaterColor



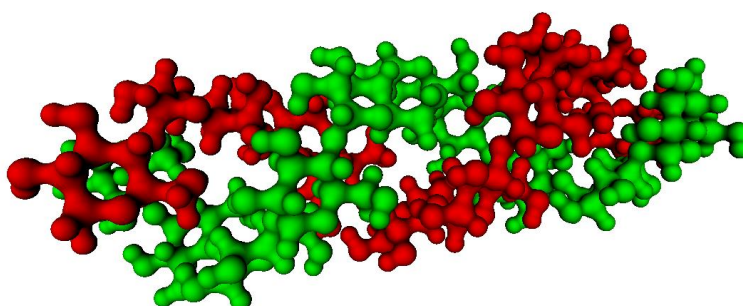
Basic



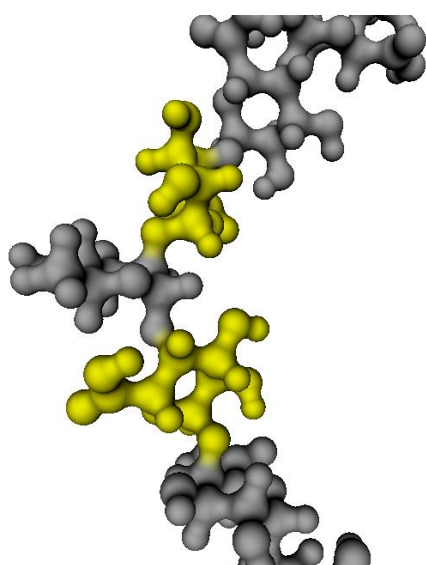
IUPAC



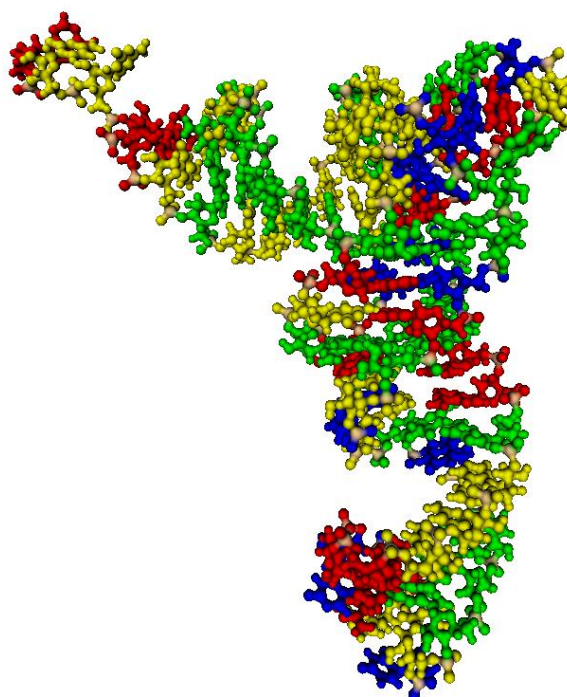
Chain



Sugar

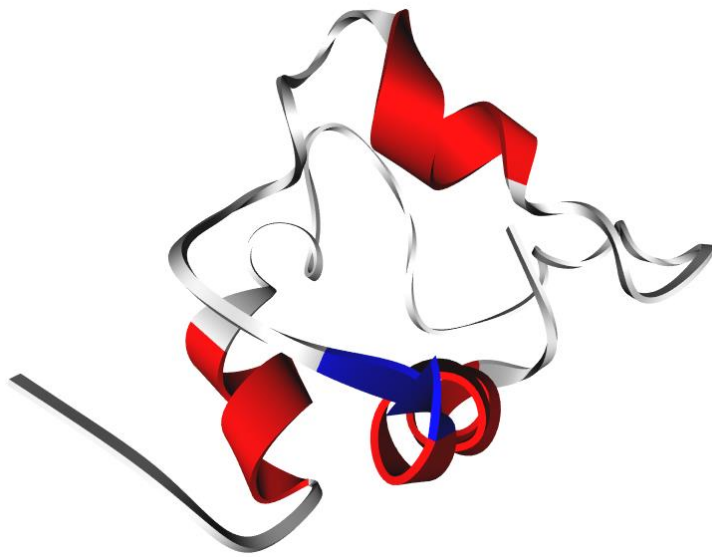


DNA/RNA

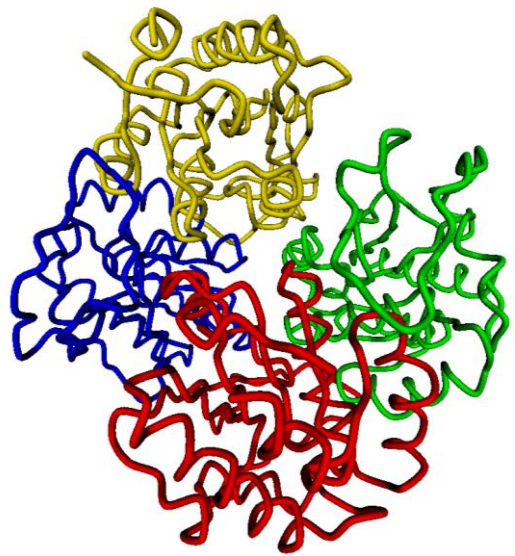


Secondary Structure Menu

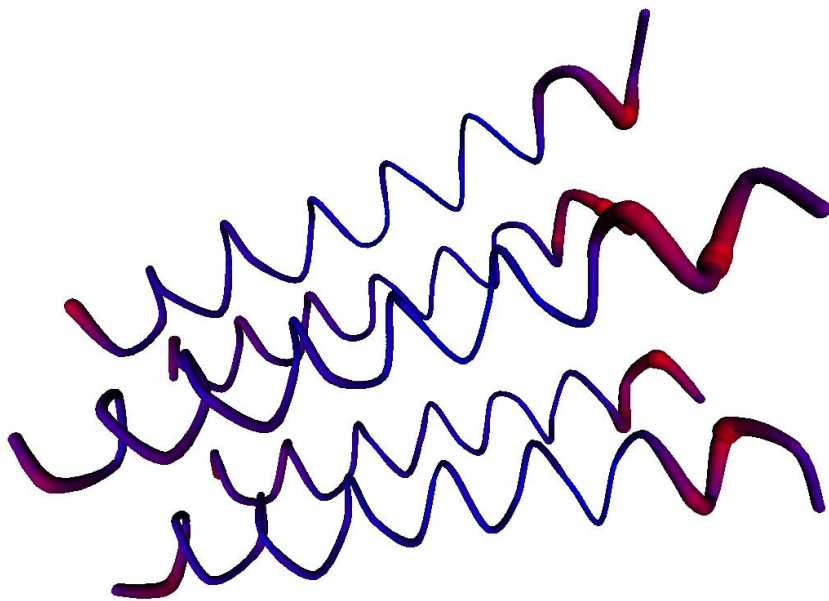
Secondary Structure



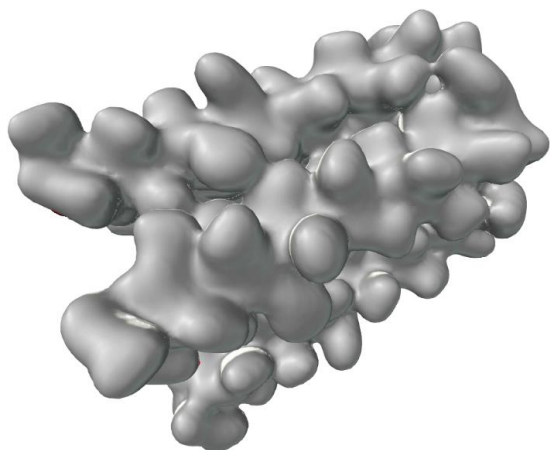
Ca-Trace



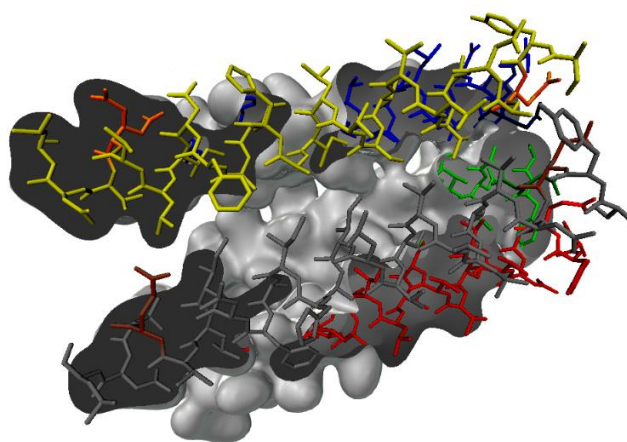
B-factor



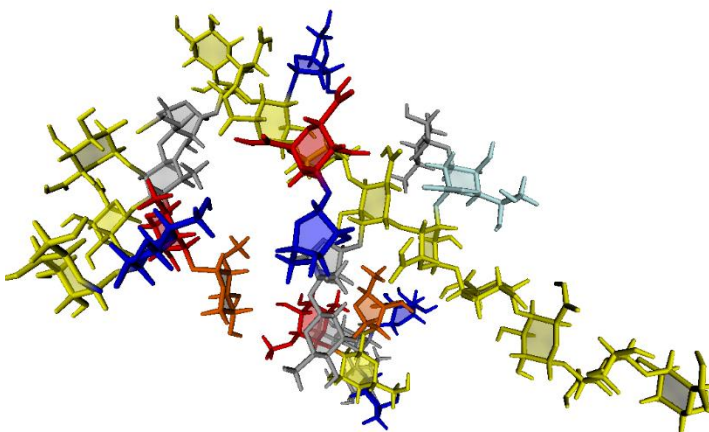
Surface mode



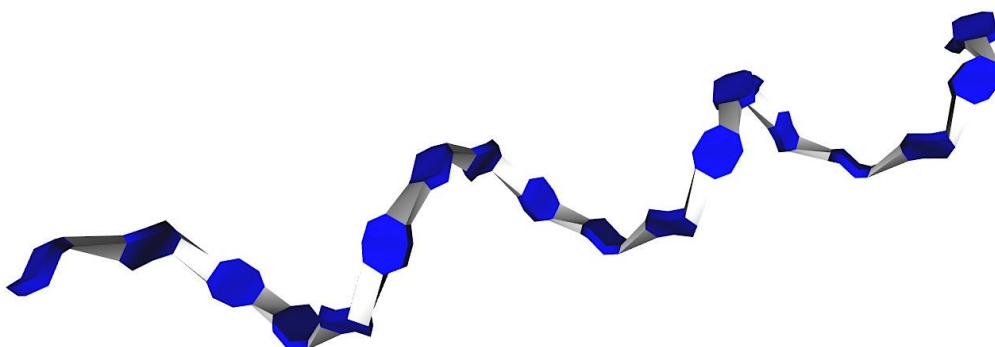
Surface with static/mobile cut



Ring
blending
(with sugar
coloration)

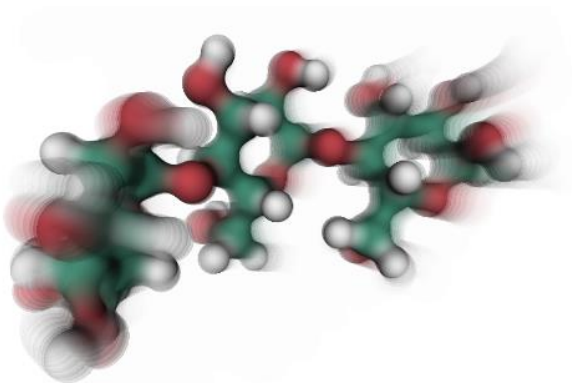


Sugar
ribbons

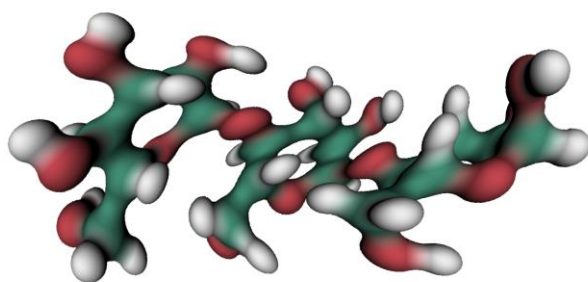


Special Effects

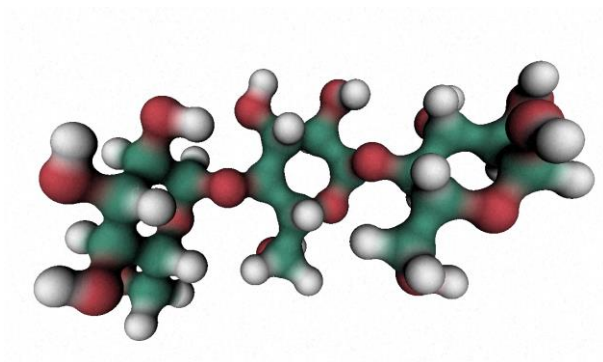
Blur



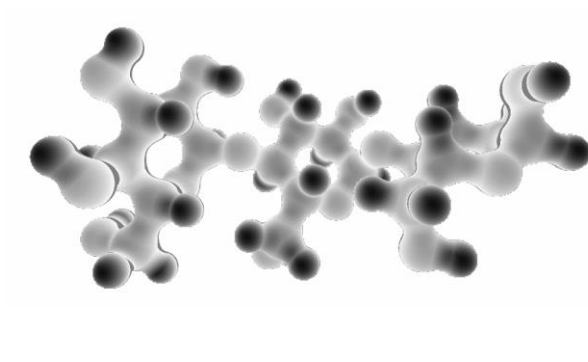
Vortex



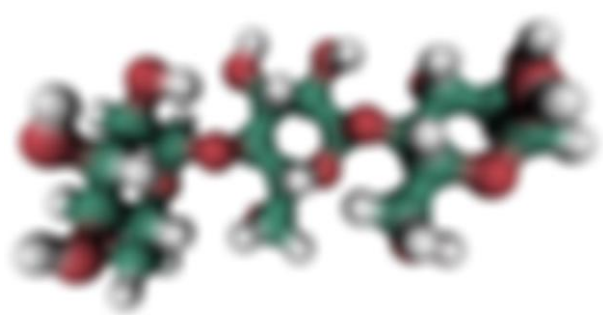
Noise



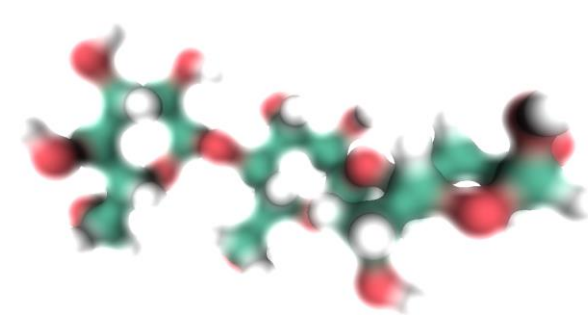
Gray



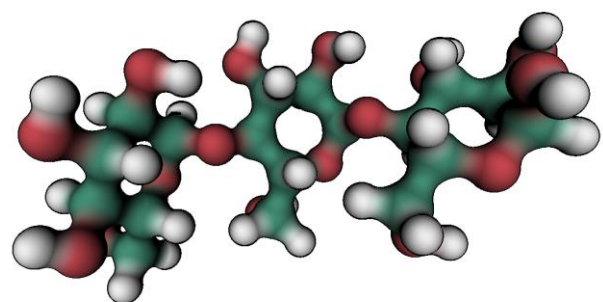
Blur2



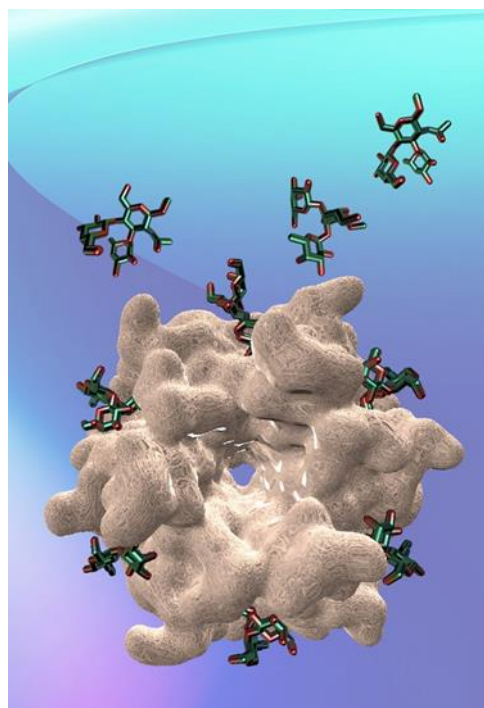
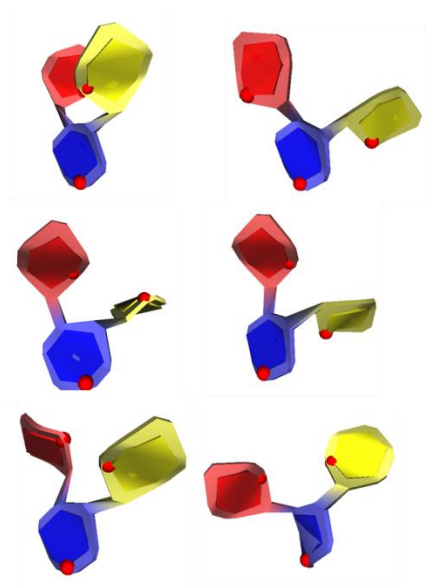
Glow



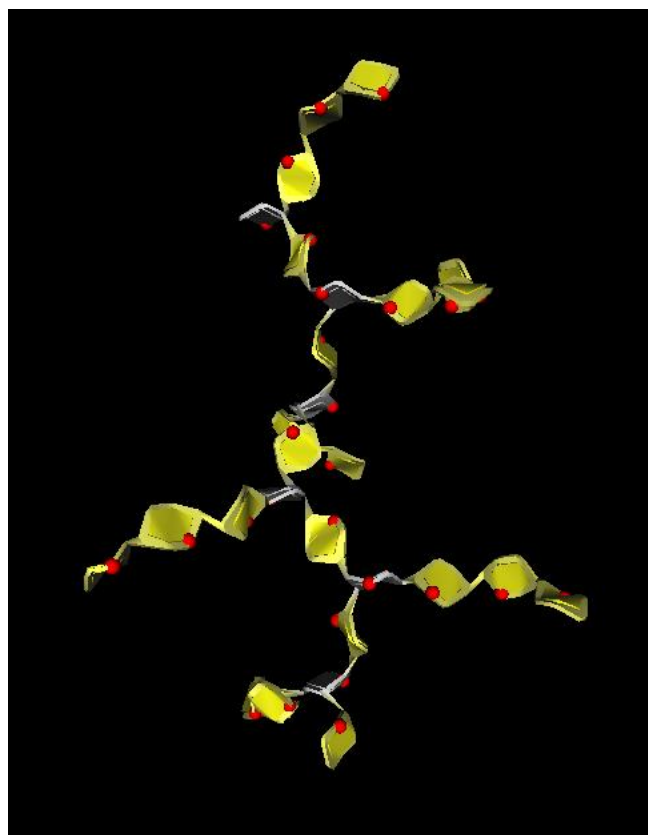
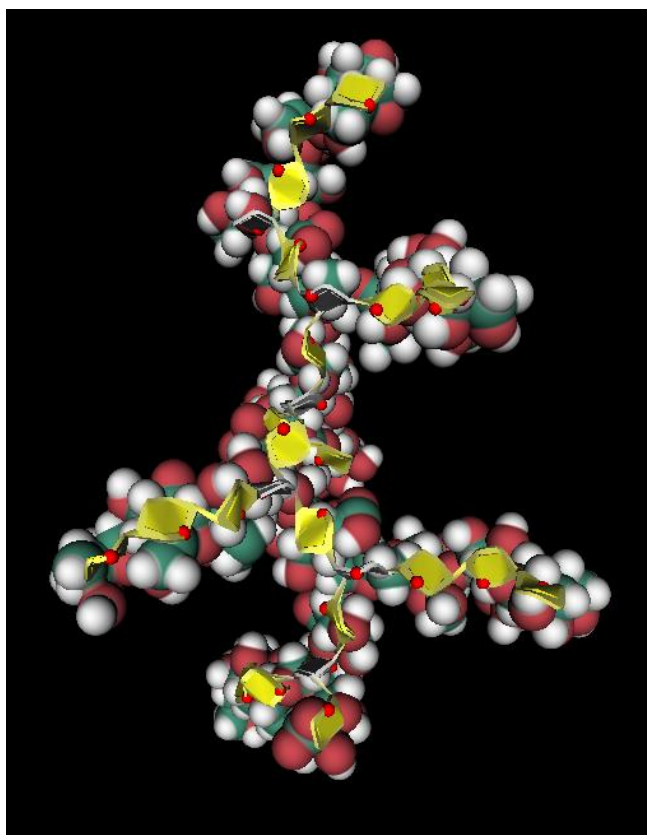
Edge



Miscellaneous



*"Coarse grain"
representation
of six low energy
conformations of
LewisX
trisaccharide
and its interaction
with a lectin;*



*Three modes of graphical representation of a complex plant polysaccharide,
making use of some of the options offered by SweetUnityMol.*